Near infrared reflectance (NIR) spectroscopy as a data supplying tool in a bio-economic approach for an optimal exploitation of sugarcane biomass

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Introduction

Sugarcane is mainly cultivated for sugar and/or first generation bioethanol production. Nonetheless, a substantial part of the sugarcane biomass remains in the fields after harvesting operations (crop residue) and generates co-products (mainly bagasse) at the sugar mill process exits. An optimal exploitation of this residual biomass is possible only through several industrial users as bioenergy (cogeneration and bioethanol) and cattle (feedstock), and/or infield uses (carbon mitigation and source of organic matter). Dispatching of components of the whole aboveground biomass to major industrial users and uses is strongly related to the harvest method and the management of the residual biomass after harvesting operations and sugar extraction process. Usually, the part of the non-harvested biomass stays in the field or goes to the cattle. The part of the harvested biomass that enters the sugar mill generates bagasse, which is mainly used for the production of energy carriers (electricity and steam). As a result it is interesting to assess bio-economic potential of sugarcane cropping-systems in regard to virtual harvesting methods and dispatching of the residual sugarcane biomass to major industrial users and uses. Multi-criteria assessment of the bio-economic potential of sugarcane cropping-systems could be based on a final common indicator (€/ha) as a unifying way to integrate complex indicators accounting for industrial users and uses environmental and economic sustainability. Complex indicators that are biologically related are quantifiable through both measurements of biochemical parameters (variables) and use of equations and/or biological models. In parallel, near infrared reflectance (NIR) spectroscopy has been widely deployed as a suitable technique for the analysis of organic components in agricultural products (Batten, 1998) as plant material (Thuriès et al. 2005; Sabatier et al. 2012) and soils (Bellon-Maurel et al. 2011). Consequently, calibration models previously developed and spectral data from sugarcane plant samples were used to predict input data (chemical characteristics) needed to run equations and/or biological models. Alternatively output data from equations and/or biological models were used to develop NIR calibrations to predict complex indicators. Finally, combined NIR spectroscopy, modelling and market values was utilised as a means to evaluate bio-economic potential of sugarcane cropping-systems.

Materials and methods

General approach

Experiments were conducted on three cultivars (R570, R579 and R585) cultivated in four-contrasted areas of la Réunion Island and harvested at five different times across plant-cane and ratoon crop cycles. Plant samples have been partitioned into five parts (millable stalk, top of the stalk, green leave blade, green leave sheath and dead leave) and each plant part was weighed fresh and dry. Plant samples were then ground with a Cyclotec™ Cyclone crusher (FOSS, Nanterre, France) to pass through a 1 mm screen and two replicates of each sample were packed into circular cups (50 mm in diameter) closed with a cardboard lid to be scanned in reflectance mode on a monochromator spectrometer (NIRSystems XDS, Inc. 7703 Montpelier Road, Suite 1, Laurel, MD 20723, USA). Spectra were obtained for each replicate at 2 nm intervals over the 400-2498 nm wavelength range. The spectra (average of 32 scans) were recorded as log 1/reflectance (log 1/R). Each sample was scanned twice (two different cup fillings) and the spectra were averaged.

Conventional analyses (van Soest (n = 228), crude fibre (n = 169), *in vitro* digestibility with pepsin and cellulase (n = 169), lower heating value (n = 169) and Dumas dry combustion (n = 56) methods) were performed on plant samples.

Based on conventional analyses and NIR measurements, several calibration models (MLR and PLS) were developed to predict quality characteristics of the sugarcane plant samples. Prediction capabilities of the calibration models were assessed by classical (for crude fibre, *in vitro* digestibility, lower heating value and Dumas dry combustion reference values) and independent cross-validation procedures (for van Soest reference values) as described by Sabatier et al. (2012). NIR predictions were then used as input data into equations and/or biological models to compute complex indicators such as electricity production capacity (EPC), feeding value for ruminants (net energy for lactation, NEL) and potential residual carbon (stable carbon or “humus”) in soils (IROC).

Computation of complex indicators

Quality characteristics as neutral detergent soluble (NDSol), neutral detergent fibre (NDF), cellulose (Cel), hemicellulose (Hem), lignin (Lig), total nitrogen (Ndumas) and carbon (Cdumas) contents, high heating value (HHV) and *in vitro* digestibility (IVD) of dried and ground sugarcane samples were used as input data to feed equations and/or biological models to predict complex indicators.

The EPC was computed based on NDF and NDSol contents, lower heating value (LHV) of the lignocellulosic compounds (Cel, Hem and Lig) from the literature (Sarlos et al. 2003) and equations given by Ripoli et al. (2000).

The NEL was calculated based on Ndumas, CF, IVD and HHV.

The IROC after sugarcane trash application was calculated according to the method described by Lashermes et al. (2009). The calculation is based on NDF, Cel, Lig and the proportion of carbon mineralized in 3 days (C3d) from trash applied to a test soil (incubation in controlled conditions), both described in the French standards for soil analysis XP U 44-162 and XP U 44-163. C3d was estimated with the TAO model (Pansu and Thuriès, 2003).

Monetization of complex indicators

Market values used to monetize the complex indicators (EPC, NEL and IROC) are given for demonstration only and are based on average prices of biomass in regard to the different industrial users and uses. The repurchase price given by Electricité de France (EDF, 2012) for electricity generated from biomass was 0.125 €/kWh. However, the price of the cattle feed ration is highly dependent of the local context and its energy concentration. In the context of la Réunion Island an average price of plant forage was set to 0.30 €/MJ of NEL. The world market value of storage C is currently around 15 €/t.

Results and discussion

NIR calibration models developed from reference values obtained by conventional analyses gave standard errors of cross-validation (SECV) and ratios performance to deviation of cross-validation (RPDcv = SD/SECV) of 1.82% (RPDcv 3.8) for NDSol, 1.94% (RPDcv 2.6) for NDF, 1.53% (RPDcv 1.9) for Hem, 1.54% (RPDcv 4.2) for Cel, 1.06% (RPDcv 1.9) for Lig, 0.15% (RPDcv 4.5) for Ndumas, 0.22% (RPDcv 7.5) for Cdumas, 3.61% (RPDcv 4.6) for IVD and 0.26 MJ kg^{-1} (RPDcv 2.2) for HHV. As a base for future work, NIR calibration models developed directly with output data from equations and/or biological models were attempted (Table 1).

Table 1. Sets description, chemometrics and model parameters and performance for electricity production capacity (EPC), net energy for lactation (NEL) and potential residual carbon in soils (IROC).

	Constituent		
Calibration set	**EPC**	**NEL**	**IROC**
Unit	kWh kg^{-1}	MJ kg^{-1}	g $100g^{-1}$
n	256	129	257
Outliers	32	3	31
Min.	1.17	2.43	14.91
Max.	1.24	5.64	34.76

Mean	1.21	4.21	24.84
SD	0.02	0.86	3.31

Table 1. Continue…

	Constituent		
Chemometrics	**EPC**	**NEL**	**IROC**
Math. treatment	D2,5,5	D2,5,5	D1,5,5
Scatter correction	SNV-D	SNV-D	SNV-D
Segments (LOO)	4	4	4
λ (range/step)	400-2498/2	800-2498/2	400-2498/2
T	13	5	12
Regression	PLS	PLS	PLS
Model parameters			
SEC	0.004	0.13	1.16
R^2c	0.92	0.97	0.88
SECV	0.005	0.15	1.22
R^2cv	0.90	0.97	0.86
RPDcv	3.2	5.7	2.7
Validation set			
n	157	39	166
Outliers	11	0	2
Min.	1.19	2.53	17.62
Max.	1.24	5.62	35.01
Mean	1.21	3.93	24.16
SD	0.01	0.98	3.68
Model performance			
SEP	0.003	0.19	1.18
R^2p	0.90	0.96	0.90
RPDp	3.7	5.2	3.1
Bias	0.002	0.05	0.73
Slope	0.98	0.98	1.03
Av. GH	0.84	1.23	0.89

n = number of samples, SD = standard deviation, LOO = leave-one-out, λ = wavelength (in nm), T = number of term, PLS = partial least square, D2,5,5 = second derivative (gap size = 5 and segment size = 5), SNV-D = standard normal variate and de-trending, SEC = standard error of calibration, R^2c = coefficient of determination of calibration, SECV = standard error of cross-validation, R^2cv = coefficient of determination of cross-validation, RPDcv = ratio performance to deviation of cross-validation (SD/SECV), SEP = standard error of prediction, R^2p = coefficient of determination of prediction, RPDp = ratio performance to deviation of prediction ($1/\sqrt{(1-R^2p)}$) as described by Dardenne, (2010) and Av. GH = average global H (Mahalanobis distances from the mean in the PLS score space).

These calibration models based on EPC, NEL and IROC estimated values (kWh kg^{-1}, MJ kg^{-1} and g $100g^{-1}$ respectively) gave standard error of prediction (SEP) and ratio performance to deviation of prediction ($RPDp = 1/\sqrt{(1-R^2p)}$ as described by Dardenne, (2010)) of $3.0*10^{-3}$ kWh kg^{-1} (RPDp 3.7), 0.19 MJ kg^{-1} (RPDp 5.2) and 1.18 g $100g^{-1}$ (RPDp 3.1) respectively. Those results are very encouraging and allow us to foresee good perspectives for this work.

The aim of this study was to present and validate an approach based on NIR spectroscopy as a supplying tool of complex indicators in a bio-economic assessment of sugarcane cropping-systems for an optimal exploitation of sugarcane biomass. Regarding the good performance of the NIR models (low SEP and fairly high RPDp), it is believed that the approach described here is suitable for the optimization of sugarcane biomass exploitation, as well as for the conception and evaluation of sugarcane cropping-systems.

As an example, a preliminary bio-economic evaluation of the sugarcane biomass exploitation through industrials users (bioenergy plant), cattle feed and infield use (stocking stable carbon or "humus" in soils) is given (Table 2). A first finding is that the value of sugarcane by-products is much more constant in energy production than for other uses: the coefficient of variation is 1.2% for energy, 18.4% for cattle feed and 12.9% for soil carbon. The bio-economic evaluation reveals that the use of bagasse in bioenergy plant for electricity production is from far the most interesting way of valorisation with roughly 5200 € ha^{-1} more incomes than for cattle feed. This statement is supported by a high repurchase price of the electricity from biomass in that typical context. However, the use of the bagasse for cattle feed can still be an alternative way of valorisation, e.g. in case of absence of bioenergy plant and/or of remoteness from the sugar mill complex.

Table 2. Bio-economic evaluation (€ ha^{-1}) of the sugarcane biomass exploitation through industrial users and infield use.

	Bioenergy plant	Cattle feed	Soil stable carbon (humus)
Bagasse	21124	15927	408
Green leaf and top	7422	8135	201
Trash	1648	1450	41

Green leaf and top biomass can generate more incomes (613 € ha^{-1} extra incomes) when it is used for cattle feed rather than bioenergy production. This extra amount of incomes could justify partitioning of the sugarcane biomass at a sugar mill level by the implementation of a cane cleaning station especially when green cane harvesting is practised. It results from the exploitation of trash biomass through both industrial users that its use for bioenergy production generates more incomes (roughly

200 € ha^{-1} extra income). Nevertheless, use of trash biomass for cattle feed is preferred in Reunion Island. Indeed, trash biomass is usually associated with soil that can end up in an increase in ashes yield at burning process and damage biomass boiler.

The potential capacity of stocking stable C (humus) in soil under sugarcane biomass components has a much lower valorisation in terms of incomes per hectare. However and especially for the trash biomass, this low amount of incomes must be balanced by the long-term agronomic benefits (maintain of soil fertility, gain of productivity, input reduction, weeds and pests control, etc.) that could ensue from mulch retention from both economic and environmental point of view. Also, it is important to notice that burning corresponds to a destruction of organic matter, while use by animals generates a by-product (faeces) which still contains a high part of stable carbon (as lignin, which is a well-known precursor of humus) which can be added to soils via manuring.

Conclusion

This paper shows the potential of NIR spectroscopy to predict quality characteristics of sugarcane biomass samples as a fast and reliable method in supplying reference values for use in equations and/or biological models. Most often they require measurement of a large number of variables and the involvement of the model developer. It is therefore believed that NIR spectroscopy could be suitable as a high-throughput method to estimate complex indicator in the aim to substitute for or facilitate the utilisation of equations and/or biological models.

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